

Indoline, 1-(2-pyridylmethyl)-  
20948-77-0 | DTXSID40175125

Model Performance

|       |      |
|-------|------|
| Model | Data |
|-------|------|

Weighted KNN model

| 5-fold CV (75%) |      | Training (75%) |      | Test (25%) |      |
|-----------------|------|----------------|------|------------|------|
| Q2              | RMSE | R2             | RMSE | R2         | RMSE |
| 0.93            | 22.5 | 0.93           | 22.1 | 0.93       | 22.1 |

## Model Results

**Predicted value:** 326 °C

**Global applicability domain:** Inside

**Local applicability domain index:** 3.91e-01

**Confidence level:** 5.02e-01

## Nearest Neighbors from the Training Set

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2-Methyl-5-nitro-1H-isoindole-  
1,3(2H)-dione

**Measured:** 361

**Predicted:** 323

Image not found

Acibenzolar-S-methyl

**Measured:** 267

**Predicted:** 295

Image not found

4,4'-Methylenebis(N,N-  
dimethylaniline)

**Measured:** 390

**Predicted:** 349

Image not found

1H-Pyrazole, 3,5-dimethyl-1-  
phenyl-

**Measured:** 273

**Predicted:** 287